EMR Study and DFT-Assisted Identification of Transient Radicals in X-Irradiated Crystalline Sucrose

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Supporting information

Table S1. Experimentally determined HF and Schonland conjugate tensors (in MHz) of U1.

		A_{iso}	A_{aniso}	Eigenvectors		
				*a**	*b*	*c*
HF tensors	H_α	-55.51	-29.83	-0.929	-0.370	0.015
			-7.66	0.254	-0.665	-0.702
			37.49	0.270	-0.649	0.712
	H_β	45.40	-5.78	0.661	-0.630	0.407
			-3.26	0.126	0.629	0.767
			9.04	-0.739	-0.456	0.495
Schonland conjugates	H_α	-55.67	-34.47	-0.855	-0.424	0.300
			5.22	-0.516	0.628	-0.583
			29.24	0.059	-0.653	-0.755
	H_β	45.36	-9.02	0.535	-0.626	0.567
			1.91	-0.071	-0.703	-0.708
			7.11	-0.842	-0.338	0.420

Figure S1. Figure illustrating the equivalence of wrong rotation sense to erroneous symmetry site assignment in monoclinic systems using the HF tensors from Table S1. The roadmap of the ENDOR line ascribed to the H_α coupling is depicted with solid lines – black for site 1 and red for site 2; the ones ascribed to the Schonland conjugate are depicted with dotted lines – black for site 1 and red for site 2. For the H_β coupling, orange lines were used for site 1 and green – for site 2; the ones ascribed to the Schonland conjugate are depicted with respectively colored dotted lines. Experimental positions of resonance lines of the H_α coupling are presented with filled blue circles and of the H_β coupling – purple cirles. Because the rotation planes do not perfectly correspond with bc, ca* and a*b, and in particular the degeneracy of the sites in the second plane is lifted, the roadmaps of the Schonland conjugate tensors do not perfectly coincide. As a result, for the α-coupling one of the tensors is clearly preferred by the fitting. For the β-coupling, the preference for one of the tensors is less clear from the fitting, but the Schonland conjugate tensors strongly deviates from the typical b-pattern (see Table S1).